Joint NSRC Workshop

Big, Deep, and Smart Data Analytics in Materials Imaging

Jointly Organized by the Five DOE Office of Science Nanoscale Science Research Centers and Held at Oak Ridge National Laboratory, Oak Ridge, TN
June 8-10, 2015
(www.cnms.ornl.gov/JointNSRC2015/)

Workshop Summary
and
Recommendations

Program Committee:
Eric Stach, Center for Functional Nanomaterials, Brookhaven National Laboratory
Jim Werner, Center for Integrated Nanotechnologies, Los Alamos National Laboratory
Dean Miller, Center for Nanoscale Materials, Argonne National Laboratory
Sergei Kalinin, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
Jim Schuck, Molecular Foundry, Lawrence Berkeley National Laboratory

Local Organizing Committee:
Hans Christen, Bobby Sumpter, Amanda Zetans, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
Workshop summary and recommendations

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Understanding and ultimately designing improved functional materials that possess complex properties will require the ability to integrate and analyze data from multiple instruments designed to probe complementary ranges of space, time, and energy. Recent advances in imaging technologies have opened the floodgates of high-visibility information in the form of multidimensional data sets. These high-resolution images and spectra conceal unexamined information on atomic positions and local functionalities, as well as their evolution with time, temperature, and applied fields. To gain the full benefits of such data sets, we must be able to effectively interrogate them for a variety of physically and chemically relevant information, develop pathways for probing local structure-property relationships, and synergistically link these results to atomistic theories (e.g., deep data analysis for scientific inference). The traditional simple graphical representation and visual inspection of such data sets are no longer sufficient to extract the most meaningful information. Advanced mathematical and computational methods are increasingly being incorporated into imaging sciences to deal with such “deep” data sets, and to combine data streams from different imaging techniques. However, many of the required mathematical or numerical tools are either lacking or not generally accessible to the imaging sciences community.

The workshop “Big, deep, and smart data in materials imaging”, jointly organized by the five Office of Science Nanoscale Science Research Centers (NSRCs) and held June 8-10, 2015 at Oak Ridge National Laboratory, brought together researchers from different imaging disciplines (electron microscopy, scanning probe microscopy, focused x-ray, neutron, atom probe tomography, chemical imaging, optical microscopies) as well as experts in mathematical/statistical/computational approaches to discuss opportunities and future needs in the integration of advanced data analytics and theory into imaging science. It provided a forum to present achievements in the various imaging disciplines with emphasis on acquisition, visualization, and analysis of multidimensional data sets, the corresponding approaches for theory-experiment matching, and novel opportunities for instrumental development enabled by the availability of high speed data analytic tools.

The workshop aimed to identify areas where advanced data analytics approaches will significantly increase the quality of information extracted from imaging data, and identify the role to be played by the NSRCs to make such approaches accessible to the user community. At the same time, the workshop identified areas in which enhanced interaction with researchers in applied mathematics, statistics, theoretical and computational sciences will be most beneficial to the imaging and materials sciences community in particular, and nanosciences in general.

The workshop far exceeded expectations on attendance: ~150 registered attendees, 33 presentations, ~50 posters. The attendees included representatives of the multiple DOE National Laboratories (LBNL, ANL, BNL, SNL, LANL, ORNL, Ames Lab, PNNL) as well as Frederick National Laboratory for Cancer Research, NIST, ARL, industry (Asylum, NewPath, Gatan, HP), and 16 universities (including Berkeley,
MIT, UWisc, UCSD, etc.). Participants included several leaders in the field, as described below and DOE program managers (Maracas, Lee) as observers. Furthermore, several of the attendees are chairing symposia at the Fall MRS meeting in Boston along a similar direction. Overall, this indicates that the area of big, deep and smart data in materials imaging is seen as a very high priority by a broad representation in the scientific community. From the content of the presentations, it became obvious that the topic of establishing data, knowledge, and skill-set connections between imaging and HPC infrastructure is evolving very rapidly, and is not limited by the introduction of new instrumentation but rather by connection between individual efforts.

Several common research topics were identified, including

1. The need for mathematical tools for imaging, especially those based on compressed sensing (LBNL, ANL, PNNL) and Markov chain models (NIST, Purdue)
2. Opportunities with ptychography (ANL and LBL for X-ray, LBL and ORNL for STEM)
3. Development of pipelines for direct data transfer from imaging tools (STEMs/XRay/SPM) to HPC (LBL, BNL, ANL, etc)
4. Direct image quantification via atomic positions (ORNL, LBL, NCSU, NIST)
5. Beam control in STEM for fats data acquisition and matter manipulation (ORNL)

We note that the selection of these topics is driven either by the physics of the imaging process (e.g., low dose imaging necessitates compressed sensing methods) or new opportunities for characterization of matter (ptychography, which effectively combines scattering and sub-atomic resolution imaging). Pursuing these directions in turn requires the development of the infrastructure (pipelines) and data analytics tools (visualization, unsupervised learning, reconstructions), in the absence of which the amount of information available for analysis is limited by human analysis and a selection bottleneck. Also noteworthy is that many of these programs have been active for extended periods of time (CAMERA at LBL for 6 years, I^3 at Argonne for 2 years, chemical imaging initiative at PNNL for ~4 years).

Workshop overview: Smart imaging of materials lets national labs look to solving big energy problems

In the Stone, Bronze and Iron Ages, the state of the art of materials science defined the zenith of technology and accelerated economies. Now, in the Information Age, data drives the development of advanced materials for energy-efficient superconducting wires, safer nuclear power plants, stronger, lighter vehicles with better batteries—and more. In this context, this workshop discussed opportunities and challenges as imaging and data sciences merge. Those efforts will likely aid the Materials Genome Initiative, which aims to speed new materials to the global marketplace.

“Combining physics with big data could produce a new field, akin to the merger of biology and engineering that created bioengineering,” said Sergei Kalinin, an organizer of the workshop and director for ORNL’s Institute for Functional Imaging of Materials.

Companies like Google and Facebook have long grappled with a volume, variety and velocity of data that characterizes it as “big.” Members of the scientific community, however, have differing degrees of experience with “big data.” Physicists sifting through mountains of data from a collider experiment to find signs of an exotic subatomic particle, for example, have more experience with it than do materials scientists examining images of a failed battery material, who often cherry-pick data related to the failure but leave the rest of the data unexamined.
That unmined data may hold vast riches. To reveal them, big data approaches must get deeper and smarter. “Deep data” strategies use theory to inform experiment and vice versa. “Smart data” tactics, on the other hand, try to do those better with unparalleled expertise and equipment.

With its big-data focus, industry isn’t advancing the deep- or smart-data approaches needed to accelerate advances in materials for energy applications. “Big data means correlation, and ignores causation,” Kalinin said. A deeper, smarter approach that merges imaging data with physical laws may allow scientists to understand the causes of problems in existing materials and predict the behaviors of designed materials. But that strategy depends on directly transferring atomically-resolved data from scanning transmission electron microscopes and X-ray experiments to high-performance computing resources for analysis and visualization.

“Facebook and Google use and re-use information already on the web. Our ground floor is to build an instrumental infrastructure that can stream data to the web,” Kalinin envisioned. “Traditionally, imaging instruments were not developed to provide uninterrupted data to the web, so only small fraction gets analyzed. We need to develop data pipelines.”

**Promising merger**

The workshop’s speakers shared promising projects that merge imaging and data sciences. “The merger allows scientists to do something deeper, but challenges remain in bringing together two philosophies,” Kalinin said. “Data is understood numerically, but imaging is not—yet.”

A looming challenge is unifying the language of microscopic data to establish common definitions for the “information content” of images. ORNL microscopist Albina Borisevich said she no longer “takes pictures” of materials but instead collects ever-increasing amounts of quantitative data from them. That data provides information about material properties and structures at atomic resolution with precision approaching that of X-ray and neutron characterization tools. Engaging advanced computational approaches brings new capabilities in data analysis, such as allowing analysis of physics and chemistry reflected in picometer-level details of images. “Cross-pollination of different imaging disciplines with computational flavor is already bringing unexpected fruit,” she said. “Implementation of the scanning-probe-like beam control allows us to use electron microscopy to fabricate the smallest 3D structures.”

Similar work is being performed at U. Wisc. by Paul Voyles, who have demonstrated the use of advanced image analytics tools to increase precision of atomic position in STEM to sub-pm. This work closely aligns with the effort of J. LeBeau of NCSU devoted ot experimental analysis of atomically-resolved images, and S. Patala applying the graph theory to image parametrization.

**James Sethian**, a mathematics professor at the University of California, Berkeley, spoke about CAMERA, a pilot project he directs at Lawrence Berkeley National Laboratory that DOE’s offices of Basic Energy Sciences (BES) and Advanced Scientific Computing Research (ASCR) support. CAMERA convenes interdisciplinary teams of mathematicians, experimental scientists and software engineers to build mathematical models and algorithms for tools critical to users of DOE facilities. “When these teams work together, they can make sense of the deluge of data, and provide the insight to turn data into information that can accelerate our scientific understanding,” he emphasized. He described work on ptychography (which combines scattering and sub-atomic resolution imaging), image analysis, chemical informatics, GISAXS (grazing-incidence small-angle X-ray scattering) and fast methods for electronic structure calculations. D. Ciston of LBL further demonstrated the use of advanced mathematical tools in the form of image libraries for fast analysis of ptychographic data in STEM.
ORNL mathematician Rick Archibald provided an overview of the ACUMEN project, funded by ASCR and focused on the mathematical challenges of scientists at the SNS and CNMS. To bring high-performance computing to the massive data sets generated by scientific experiments at ORNL, ACUMEN’s partners develop next-generation algorithms for scalable analytics. M. Demkovicz of MIT delineated the use of Bayesian methods for analysis of the image data and reducing it to materials specific parameters.

“Powerful imaging techniques demand increasingly large bursts of computing power to drive their data analysis,” said David Skinner, who leads strategic partnerships between the National Energy Research Scientific Computing Center (a DOE Office of Science User Facility at Lawrence Berkeley National Laboratory) and research communities, instrument/experiment data science teams and the private sector. “Accessing shared high-performance computing through fast networks is an increasingly interesting prospect for these data-driven instruments.”

ORNL software engineer Eric Lingerfelt described the Bellerophon Environment for Analysis of Materials (BEAM) software system, which will, for the first time, enable instrument scientists at CNMS to leverage ORNL’s powerful computational platform to perform near real-time data analysis of experimental data in parallel using a web-deliverable, cross-platform Java application. The BEAM system also offers robust long-term data management services and the ability to transmit data files over ORNL’s high-speed network directly to CADES. “BEAM users can easily manipulate remote directories and data in their private storage area on CADES as if they were browsing their local workstation,” Lingerfelt said. Similar effort is being undertaken by F. Ogletree and his team at LBL.

Managing unprecedented data streams is a big challenge. Fortunately, colocation of NSRCs with other facilities grappling with this elephantine issue gives DOE nanocenters a huge advantage in finding solutions. RHIC, an accelerator at Brookhaven National Laboratory (BNL) looking at the quark gluon plasma, and ATLAS, a detector at CERN’s Large Hadron Collider, are both high-energy physics projects that generate lots of data. The RHIC & ATLAS Computing Facility at BNL manages the data for both. Eric Stach, who leads the Electron Microscopy Group in the Center for Functional Nanomaterials at BNL, noted that the RHIC/ATLAS detector curated 160 petabytes of data in 2013, and will surpass 200 petabytes this year. So materials scientists have learned a lot from nearby physicists—a boon because a single STEM instrument can produce a data flow similar to that of the ATLAS detector, Kalinin interjected. Said Stach, “The introduction of sensitive new detectors and ultra-bright sources is leading to an explosion of rich materials data—we expect to have more than 20 petabytes generated each year at the user facilities at Brookhaven. That’s the data equivalent of one-fifth of every Google search done in 2013.”

Nigel Browning of Pacific Northwest National Laboratory (PNNL) described methods, statistics and algorithms to extract information from images obtained using aberration corrected electron microscopy, which enables very high resolution images of increased data quality and quantity. Compressive sensing, for example, pays attention to bits of a sample and uses signal processing to fill in the blanks. Kerstin Kleese van Dam, then of PNNL (now at BNL), spoke about streaming analysis of dynamic imaging experiments that promise to capture evolving processes in materials under operating conditions.

Big data and mathematical methods can build the bridge needed to link theory to experiment, Kalinin said. One problem has been data takes longer to process (e.g., a month on an 8-core computer) than acquire time (say, 10 hours). For ORNL’s Borisevich, that problem had a solution. They acquired ultrafast data from STEM and piped it directly to the Titan supercomputer—which has 299,008 CPU cores to guide simulations while accompanying GPUs handle hundreds of calculations simultaneously—for analysis.
Experiment and theory work hand in hand to show how the real structure and function of a material compare to the ideal. Experiment helps inform and validate theory and theory-based models. “Highly resolved imaging techniques give information about atoms that need to be put into the theory. Then a model based on theory can tell properties. You can make inferences from that information,” according to ORNL theorist Bobby Sumpter. “Theory can connect pieces given from experiment, such as physics and mechanical properties and how they change upon for instance, introducing a dopant. You can fill in information and complete the story and move forward to ask, how can we make materials better?”

Whereas microscopy gives information about the surface of a material, neutron scattering digs deeper to give information about the bulk material. Combining the two can inform theories and models for predicting properties of designed materials, according to Sumpter. Kalinin said, “Once we have the infrastructure to stream our data from microscopes and we can measure structures and properties, we can start to build libraries of structure–property relationships on the single-defect level. We can verify libraries against X-ray and neutron scattering methods and know if a library is complete.”

Combining multimodal experiment and theory advances the advent of materials by design. “This is the first time in history we’ve matched experiment with theory,” Sumpter said. “We should have some success.” Success may mean understanding structural deviations called “defects” in atomically ordered materials. “Defects are not doom if you understand what they are and do,” Sumpter said. ORNL’s Thomas Proffen works at SNS, which provides the world’s most intense pulsed neutron beams for scientific research and industrial development. This accelerator-based neutron source is next-door to CNMS and has approximately 20 beamline experiments that measure structures and dynamics of materials in diverse applications from biology to additive manufacturing. The data sets are huge. “Neutron data has a lifecycle from the time the neutron hits the detector to the identification of scientifically interesting data,” Proffen said. “When data sets are small, people can keep on top of it. Now we can’t.”

Proffen is the director of the neutron data analysis and visualization division in the Neutron Sciences Directorate of ORNL and also heads the Center for Accelerating Materials Modeling (CAMM), funded by BES specifically for direct integration of simulation and modeling into the analysis loop for data from neutron experiments. Direct integration allows scientists to refine theoretical models against experimental observations, use models to predict where new experimental measurements should be performed, and analyze some data at the user facility before taking it to the home institution for full analysis. “Neutron events are streamed and processed live, allowing a near-real-time view of collected data so a scientist running the experiment can make decisions on the fly,” Proffen said. “To visualize data, we play with everything from virtual reality headsets to volume rendering on parallelized servers.”

At Supercomputing 2014, ORNL researchers demonstrated the pipeline for diffuse scattering data of material defects. Through CAMM, researchers identify existing computational methods, such as pattern recognition and machine learning, providing new ways to extract data. If brute-force computing is to help process data from neutron scattering, Proffen said, future challenges include managing metadata (“data about data”), handling instrument and experiment configurations, and planning tools.

Scientists are producing so much data that the majority goes unanalyzed, according to Thomas Potok, who heads ORNL’s Computational Data Analytics group and led an automation project identifying research papers made possible through use of ORNL’s supercomputer to provide a metric of its scientific impact. Noting that data is published in papers that are the primary output of science, Kalinin asked Potok: Is there a better way to exploit papers to make additional discoveries? Potok set up automated tools that in part assigned greater weight to papers with higher impact factors and used them to find interesting papers, “in the Amazon sense of a ‘recommend’: ‘Hey! You bought this. Maybe you want
this?’ Look at some recommendations and you say, ‘These people may be valuable to bring in to my next workshop.’”

The next step for text analytics is deep learning, which relies on computing. “The exciting thing is deep learning has made a lot of breakthroughs using GPUs,” Potok said. “At Stanford they were able to recognize cat faces using a cluster of 64 GPUs. Well, we’ve got this Titan computer that’s got 18,000 GPUs.” National labs could deftly adopt off-the-shelf technologies to interpret imaging data in the form of text, including chemical and mathematical formulae, according to Kalinin.

During a meeting break, Chad Steed of ORNL entertained questions about data visualization, which processes data that is copious and complex. “We’re combining computational analytics with interactive data visualization—the human part—so that we could bring in scientists’ intuition and their background knowledge that you [might] lose with a purely data analytics approach,” he said. A visual analytics system could essentially look over a scientist’s shoulder and engage algorithms that learn from the scientist’s interactions and improve its ability to predict what the scientist thinks is interesting. “It could build up a knowledge repository that a novice could use to start up with at least some of the initial capabilities of an expert scientist,” Steed said. “Humans are very good at visual processing and intuition tasks that are hard to do with a computer. If we could grasp that strength of the humans in some type of intelligent interface, we could go after problems that neither approach in isolation could solve.”

**Discussing the path forward**
The meeting concluded with a panel discussion, moderated by CNMS’s Christen, of what DOE’s nanoscience centers can and should do to help the scientific community strengthen the link between data and imaging sciences.

“We’re transitioning from imaging being a qualitative tool to a quantitative tool,” Kalinin pointed out. “This requires hardware platforms, and lo and behold because of the previous investment made by DOE and other funding agencies, these platforms exist. These platforms happen to be extremely data-intensive in terms of data generation and extremely demanding in terms of analytics. And at the same time we have all the capabilities enabled by supercomputing. This feels like a perfect storm.”

To use knowledge from imaging to improve predictive theories, scientists need a proper mathematical framework implemented on machines they can use, Kalinin said.

Stach of Brookhaven’s Center for Functional Nanomaterials said the lack of staff specifically associated with data management and data methods was a problem. “We don’t have a central resource (for users and staff) where there’s deep expertise in these areas,” he said. Having on-board experts acting as liaisons to centers at the forefront of the big-data tsunami, such as light and neutron sources, could spur opportunities to gain knowledge of best practices and incorporate different approaches.

“We’re still at the place where there’s a lot of ‘artisanal software’ being put together,” said James Shuck, director of Imaging and Manipulation of Nanostructures Facility at Berkeley’s Molecular Foundry. “This is where we need people to start talking to one another. The data modeling people are starting to talk to the data generators; that’s key. However, there’s still plenty of jargon, which is a sign they’re half talking past each other.” The solution is having people who spend their time thinking about this. “This is an opportunity DOE and the NSRCs have. There’s a reason the NSRCs are at the labs. It’s because they are colocalized with other facilities. There’s a chance for real interaction to occur.”
Dean Miller of Argonne’s Center for Nanoscale Materials agreed, emphasizing the need for standardized data formats. “We need teamwork,” he said. “Vendors may have a proprietary format, but we can push them to make sure that their software will provide the data in an open-source data format as well.”

Miller said his electron microscopy center is collocated with other facilities at the forefront of big-data management. “We’re benefitting tremendously from [researchers at the collocated Advanced Photon Source] tackling many of these problems,” he said. As the nation’s nanocenters were built, community involvement and participation from other facilities were critical. “In terms of now addressing these challenges for data, that same strategy holds: We need community involvement to guide us.”

“We absolutely need to be doing continuous education,” Kalinin of Oak Ridge’s IFIM said to an audience and panel enthusiastic about the suggestion. He cited the success of specialized “boot camp” workshops, e.g. in computing topics. “Those of us who got PhDs 10 years ago or more have very limited if any clue about the power of the modern statistical methods—computation and so on. As part of our regular job routine, the chances of doing it are remote,” he said. “Without this, we simply won’t be able to learn tools in the areas which are vital to us.”

A university professor in the audience said, “I push my students, but they don’t have the tools to use.” She suggested students and teachers as well as scientists could benefit from boot-camp-style online teaching modules. Stach praised the National Science Foundation’s nanoHUB tool to disseminate computer programs helpful in nanoscience and nanotechnology. “The effectiveness of online education is very clear,” he said.

Shuck confessed awe at the fact that a colleague can take 3D tomographs, and while the experiment is ongoing, analyze and reconstruct the data in multiple ways and reask questions. “I couldn’t do that three years ago. We’ve seen knowledge accelerate,” he said. “If a tutorial is made, I’d like to take that class.” He pointed out that many attendees of the DOE nanoscience-centers workshop were also planners of an data-related symposium at the upcoming meeting of the Materials Research Society and could suggest workshops or tutorials to benefit the broader community.

Original story by Dawn Levy:

CAPTION/CREDIT: The “Big, Deep and Smart Data Analytics in Materials Imaging” workshop included a welcome from ORNL’s Michelle Buchanan (top left), activities (top right) and poster sessions (bottom left) at which researchers could share findings as well as panel discussions (bottom right, with from left, Oak Ridge’s Hans Christen, Brookhaven’s Eric Stach, Berkeley’s James Shuck, Argonne’s Dean Miller, and Oak Ridge’s Sergei Kalinin.) Image credit: Oak Ridge National Laboratory, U.S. Dept. of Energy; photographer Genevieve Martin, photo collage Allison Gray
Workshop Recommendations

1. Integrated tool development: Based on the workshop, several common research topics were delineated, including
   1. Mathematical tools for imaging, especially those based on compressed sensing (LBNL, ANL, PNNL) and Markov chain models (NIST, Purdue)
   2. Ptychography (ANL and LBL for X-ray, LBL and ORNL for STEM)
   3. Pipelines for direct data transfer from STEMs/XRay to HPC (LBL, BNL, ANL, etc)
   4. Direct image quantification via atomic positions (ORNL, NCSU, NIST)
We note that the selection of these topics is driven by the physics of the imaging process (e.g., low dose imaging necessitates compressed sensing methods) or new opportunities for characterization of matter (ptychography, which effectively combines scattering and sub-atomic resolution imaging). Pursuing these directions in turn requires the development of the infrastructure (pipelines) and data analytics tools (visualization, unsupervised learning, reconstructions), in the absence of which the amount of information available for analysis is limited by human analysis and a selection bottleneck.

For these common topics, we recommend the integration of the software development effort across the NSRCs (and potentially beyond), including:
   - Establishing common file format and systems for storing metadata
   - Establishing universal code repository, e.g. based on GitHub
   - Development of integrative platforms that allow cross-checking of the codes from different group and their availability for broad community via app-like system
The specific pathway to achieve this goal can be via informal meetings among PIs followed by the software development hackathons to establish the synergy in software development effort between the groups.

2. Cloud Imaging: The emergence of high-resolution aberration corrected imaging and ptychography in synergy with big data techniques signifies a paradigm shift of electron microscopy from imaging to quantitative structural tool much like synchrotrons and scattering facilities. Unlike the scattering facilities, this Big Data STEM infrastructure is likely to rely on distributed network of instrumental facilities and data analytics (imaging in the cloud). We believe that presently the field is posed on the brink of the fundamental paradigm change enabled by confluence of high-resolution imaging and full harnessing of information flow from the microscope, specifically by recording the complete scattering distribution at atomic resolution. The confluence of recent advances in instrumentation, detectors, and computing power will enable widespread adoption of ptychographic imaging as a universal STEM imaging mode, as a next paradigm beyond aberration-corrected imaging. Even though data generation rate for STEM in ptychographic mode can be comparable to that of the LHC, fully harnessing this data flow has the potential to revolutionize our capability to probe the structure and functionality of matter in 3D and with sub-atomic resolution. Among the benefits:
   - Lateral “super-resolution” - because images are not generated in the conventional manner, the usual resolution limits do not apply, allowing the extraction of structural information beyond existing barriers and potentially pushing information limit by an order of magnitude.
   - Vertical super-resolution – just like in holography, the three-dimensional information is encoded in the dataset, which should allow characterization of all the atoms in a three-dimensional structure.
   - Electrical and magnetic field data recovery without specialized probes or microscopes – approaches such as electron holography use sophisticated illumination schemes to partly recover the electron phase lost in integration on the detector. With a ptychographic data set, retrieving this information becomes a software, rather than a hardware, problem.
- Imaging physics – the goal is to extract as much information as possible from every electron. Phase determination will allow computational reconstruction of sample characteristics and refinement of the models of beam/matter interactions. Multiple detectors can be numerically applied, allowing all of the conventional images to be reconstructed from a single dataset. Unique numerical detector geometries optimized for specific properties that cannot be implemented in hardware can be applied this way.

- Combination with electron energy loss spectroscopy or other spectroscopy techniques holds as-yet unexplored potential.

To implement these aims, a targeted investment into better detector systems for the existing microscopes will be required across the board, including potential development of novel detection devices. This will result in massive increases in data volumes, which will in turn require advanced computing resources to store and to process the data. Pipelines from imaging instruments to advanced computing power, including development of software and mathematical tools, would have to be included. We envision a distributed infrastructure for data acquisition and analysis that would integrate imaging instruments and advanced computing resources. Such a system should ensure web-openness to other users and theorists, and comply with new regulatory requirements.
Appendix A: Initial ad

NSRC Workshop “Big, deep, and smart data in materials imaging”

Jointly organized by the five Office of Science Nanoscale Science Research Centers
June 8-10, 2015 at Oak Ridge National Laboratory, Oak Ridge, TN

Organizing Committee:
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Jim Schuck, Molecular Foundry, Lawrence Berkeley National Laboratory

Point of contact: Amanda Zetans, zetansac@ornl.gov

Background: Understanding and ultimately designing improved functional materials that possess complex properties will require the ability to integrate and analyze data from multiple instruments designed to probe complementary ranges of space, time, and energy. Recent advances in imaging technologies have opened the floodgates of high-veracity information in the form of multidimensional data sets. These high-resolution images and spectra conceal unexamined information on atomic positions and local functionalities, as well as their evolution with time, temperature, and applied fields. To gain the full benefits of such data sets, we must be able to effectively interrogate them for a variety of physically and chemically relevant information, develop pathways for probing local structure-property relationships, and to synergistically link these results to atomistic theories (e.g., deep data analysis for scientific inference). The traditional simple graphical representation and visual inspection of such data sets are no longer sufficient to extract the most meaningful information. Advanced mathematical and computational methods are increasingly being incorporated into imaging sciences to deal with such “deep” data sets, and to combine data streams from different imaging techniques. However, many of the required mathematical or numerical tools are either lacking or not generally accessible to the imaging sciences community.

Scope: This workshop will bring together researchers from different imaging disciplines (electron microscopy, scanning probe microscopy, focused x-ray, neutron, atom probe tomography, chemical imaging, optical microscopies) as well as experts in mathematical/statistical/computational approaches to discuss opportunities and future needs in the integration of advanced data analytics and theory into imaging science. It will provide a forum to present achievements in the various imaging disciplines with emphasis on acquisition, visualization, and analysis of multidimensional data sets, the corresponding approaches for theory-experiment matching, and novel opportunities for instrumental development enabled by the availability of high speed data analytic tools.

Outcomes: The workshop aims to identify areas where advanced data analytics approaches will significantly increase the quality of information extracted from imaging data, and identify the role to be played by the NSRCs to make such approaches accessible to the user community. At the same time, the workshop will identify areas in which enhanced interaction with researchers in applied mathematics, statistics, theoretical and computational sciences will be most beneficial to the imaging and materials sciences community in particular, and nanosciences in general.

Format: The workshop will consist of plenary lectures to introduce the key areas of interest, contributed talks and posters, as well as panel discussions and breakout sessions to discuss the needs and opportunities in the various areas.
Tentative Topics include:

- Unsupervised learning for image analysis, classification, and information extraction
- Harnessing structural and functional imaging for materials development and discovery, for soft/hybrid as well as for hard materials
- Deep learning in imaging: Bayesian inference, parameter space compression, exploring unstructured data
- Integrating data sets from different imaging modalities and different length and time scales
Appendix B: Program

Joint NSR Workshop – Big, Deep, and Smart Data Analytics in Materials Imaging

Program

(p): Plenary lecture, 45 min., including questions  
(i): Invited talk, 30 min., including questions  
(c): Contributed talk, 15 min., including questions  
(d): Panel discussion, 30 min.

Monday, June 8:

7:30 – 8:15 Breakfast

8:15 – 8:30 Introduction (M. Buchanan, ORNL Associate Laboratory Director for Physical Sciences)

8:30 – 8:45 Introduction (J. Nichols, ORNL Associate Laboratory Director for Computational Sciences)

8:45 – 9:00 Introduction (H.M. Christen, Director, Center for Nanophase Materials Sciences)

9:00 – 10:30 Morning session 1

• T1 (p): J. Sethian (Berkeley), CAMERA: The Center for Advanced Mathematics for Energy Research Applications
• T2 (i): I. McNulty (ANL), TBD
• T3 (c): T. Potok (ORNL), Beyond Gutenberg: A Computational Analysis Approach to Scientific Discovery and Innovation

10:30 – 11:00 Coffee Break

11:00 – 12:30 Morning session 2

• T4 (i): E. Stach (BNL), Creating a Big Data Ecosystem at the Brookhaven National Laboratory: Successes, challenges and needs
• T6 (i): D. Vine (ANL), Real time phase retrieval in nanobeam ptychography

12:30- 2:30 Lunch/poster session
2:30 – 4:00 Afternoon session 1
- T7 (i): P. Voyles (U. Wisc), Extracting Materials Structure Knowledge from STEM Data
- T8 (i): D. Ushizima (LBL), Scaling Analytics for Image-based Experimental Data
- (d) Panel session (B. MacCabe [Chair], J. Ciston, E. Stach, F. DeCarlo), Big data infrastructure for Imaging – challenges and opportunities

4:00 – 4:30 Coffee Break

4:30 – 5:45 Afternoon session 2
- T9 (i): Q. Chen (UIUC), Insights from watching dynamics: from patchy spheres to anisotropic nanocrystals
- T10 (c): B. Doughty (ORNL), Reducing the Complexity of Ultrafast Transient Absorption Microscopy Data into Decay Associated Amplitude Maps
- T11 (c): M. Drouhard (UTK), Immersion Data Visualization using the Oculus Rift with Applications in Materials Science
- T12 (c): M.A. Groeber (AFRL) - DREAM.3D: Thoughts & Lessons Learned While Creating a Common Environment to Store, Share &Work With Digital Microstructure Data

6:30 Dinner (by reservation only – Riverside Grill, 100 Melton Lake Peninsula, Oak Ridge, TN 37830)

Tuesday, June 9

7:30 – 8:30 Breakfast

8:30 – 10:30 Morning session 1
- T13 (i): S. Sankaranarayanan (ANL), Imaging and visualizing ultrafast energy transport via molecular simulations
- T14 (i): D. Skinner (LBL), Design Patterns in Web-based HPC : Materials Imaging
- T15 (i): T. Proffen (ORNL), Neutrons, Materials and Data Challenges
- (d) Panel session (B. Sumpter [Chair], S. Sankaranarayanan, D. Skinner, P. Kotula ) Linking big data to computing for materials design

10:30 – 11:00 Coffee

11:00 – 12:30 Morning session 2
- T16 (i): K. Kleese van Dam (PNNL), Towards streaming analysis of dynamic imaging experiments
- T17 (c): E. Lagerfeld (ORNL), A New Computational Infrastructure for the Advanced Analysis of Nanophase Materials Imaging
- T18 (c): W.C. Yang (NIST), Automatic Image Analysis of High Resolution Videos Obtained Using Environmental Transmission Electron Microscopy
• T19 (i): N. Browning (PNNL), *Using Compressive Sensing, Statistics and Automated Tracking Algorithms to Optimize Data Acquisition in High-Resolution In-Situ TEM experiments*

12:30- 2:30 Lunch/poster session

2:30 – 3:45 Afternoon session 1
• T20 (i): M.J. Demkowicz (MIT), *Bringing Bayesian methods into the materials modeling mainstream*
• T21 (c): Rick Archibald (ORNL), *Sparse sampling methods for image processing and data analysis*
• T22 (c): M. Comer (Purdue), *Stochastic Modeling for Materials Images*
• T23 (c): M. Comer (Purdue), *Large-Scale Deep Learning for Scientific Discovery*

3:45 – 4:15 Coffee

4:15 – 5:45 Afternoon session 2
• T24 (i): A. Borisevich (ORNL), *Discovering Materials Physics in Real Space by STEM*
• T25 (i): J. LeBeau (NCSU), *Quantifying the whole STEM image: where we are and where to go from here*
• (d) Panel session (M. Demkowicz [Chair], S. Kalinin, K. Kleese van Dam, J. LeBeau ) *Inverse problems and Bayesian inference in image analysis*

6:30 Dinner (on your own)

**Wednesday, June 10:**

7:30 – 8:30 Breakfast

8:30 – 10:30 Morning session 1
• T26 (i): A. Lupini (ORNL), *Electron Ptychography in STEM*
• T27 (c): S. Patala (NCSU), *Identification of Atomic Clusters through Point-Pattern Matching Algorithms*
• T28 (c): D. Frank Ogletree (Berkeley), *Smart Imaging With Scanned Electrons*
• T29 (i): P. Kotula (Sandia), *Acquisition, Analysis and Quantification of Hyperspectral Images*
• T30 (i): D. Gursoy (ANL), *Compressive sampling and its potentials in nanoimaging*

10:30 – 11:00 Coffee

11:00 – 12:30 Morning session 2
• T31 (i): F. DeCarlo (Argonne), *Data intensive science at synchrotron based 3D X-ray imaging facilities: the Argonne National Laboratory experience from data-limited to data-intensive to data-driven science*
• T32 (c): L. Drummy (AFRL), *Data Analytics in Materials Characterization at AFRL*
• T33 (c): S.V. Kalinin (ORNL), *Big data in SPM*
(d) Panel session (H. Christen [Chair], E. Stach, D. Miller, J. Schuck, S. Kalinin) Role of NSRCs in integration of big data and imaging: science and user programs
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